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# Scalable Hybrid Deterministic/Monte Carlo Neutronics Simulations in Two Space Dimensions

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***Abstract*—In this paper we discuss a parallel hybrid deterministic/Monte Carlo (MC) method for the solution of the neutron transport equation in two space dimensions. The algorithm uses an NDA formulation of the transport equation, with a MC solver for the high-order equation. The scalability arises from the concentration of work in the MC phase of the algorithm, while the overall run-time is a consequence of the deterministic phase.**

***Keywords*-Neutron Transport, Jacobian-Free Newton-Krylov, NDA, Monte Carlo**

## I. Introduction

In this paper we report new scalability results for a hybrid deterministic/MC algorithm for the multigroup $k$-eigenvalue problem in neutron transport in two space dimensions. Our hybrid deterministic/MC solver [1], [2] is based on the Nonlinear Diffusion Acceleration (NDA) formulation of the problem [3]. The new features of the solver, as described in [1], [2] are faster and more accurate Jacobian-vector products and the use of MC simulation for the transport sweeps.

The equation is

$$\begin{aligned}\hat{\Omega} \quad &\cdot\nabla\psi_g(\hat{\Omega},\vec{r}) + \Sigma_{t,g}\psi_g(\hat{\Omega},\vec{r}) \\ &= \tfrac{1}{4\pi}\textstyle\sum_{g'=1}^{G}\Sigma_s^{g'\to g}\phi_{g'}(\vec{r}) \\ &\quad + \tfrac{\chi_g}{4\pi k_{eff}}\textstyle\sum_{g'=1}^{G}\nu\Sigma_{f,g'}\phi_{g'}(\vec{r}),\end{aligned} \tag{1}$$

with appropriate boundary conditions. This is a generalized eigenvalue problem. We are interested in the dominant (largest) eigenvalue $k_{eff}$ and corresponding eigenfunction.

In (1), $\vec{r}\in\mathcal{D}\subset R^3$, $\psi_g$ is the group angular flux and $\phi_g = \int_{4\pi}\psi_g d\Omega$ is the group scalar flux for groups $g = 1,\cdots,G$. $\Sigma_{t,g}$, $\Sigma_s^{g'\to g}$, and $\Sigma_{f,g}$ are the total, inscattering and fission cross-sections for group $g$. $\chi_g$ is the fission spectrum, and $\nu$ is the mean number of neutrons emitted per fission event.

There has been much recent work on Jacobian-free Newton-Krylov and hybrid deterministic/MC algorithms for the $k$-eigenvalue problem [1]–[8]. This paper is part of that activity.

In the remainder of the paper we briefly describe the hybrid NDA formulation of the problem in § II. We refer to [1]–[4], [6] for details and descriptions of discretizations and boundary conditions. Our interest here is parallel performance, and in § III we report on new scalablity for a problem in two space dimensions.

## II. Algorithms

The Nonlinear Diffusion Acceleration (NDA) algorithm reformulates the problem as a nonlinear equation for the group scalar fluxes [9]. In NDA, as with other nonlinear accelerators, [9]–[13], we express the fixed point problem for the flux into a "low-order" nonlinear diffusion equation. The low-order equation is coupled to the "high-order" transport equation to enforce consistency. The high-order equation is a fixed-source problem with no scattering, and is therefore easier to solve with a MC approach than the original transport equation [1], [2], [14]–[17].

As is standard, we will express (1) in operator notation as

$$\mathcal{L}\Psi = \mathcal{M}\left[\mathcal{S} + \frac{1}{k_{eff}}\mathcal{F}\right]\Phi. \tag{2}$$

In (2), $\mathcal{L} = \hat{\Omega}\cdot\nabla + \Sigma_t$, $\mathcal{M} = \frac{1}{4\pi}$, $\mathcal{S} = \Sigma_s$, and

$$\mathcal{F} = \chi\nu\Sigma_f.$$

$\Psi$ is the vector of group angular fluxes, and $\Phi$ is the vector of group scalar fluxes. A simple power method iteration can converge very slowly. The NDA formulation will converge more rapidly.

NDA splits the transport problem into a "high-order" transport problem with no scattering in the right side of the equation and a "low-order" diffusion equation. The resulting system of equations is nonlinear, but iterative methods converge more rapidly for the NDA system than for the original problem [3], [9]. We will express the NDA formulation as a eigenvalue problem for the low-order flux $\Phi$.

Given $\Phi$ and $k_{eff}$, we compute a high-order angular flux $\Psi^{HO}$, scalar flux $\Phi^{HO}$, and current $J^{HO}$ by

$$\begin{aligned}\Psi^{HO} &= \mathcal{L}^{-1}\mathcal{M}\left[\mathcal{S} + \frac{1}{k_{eff}}\mathcal{F}\right]\Phi, \\ \Phi^{HO} &= \int\Psi^{HO}d\hat{\Omega}, \\ \vec{J}^{HO} &= \int\hat{\Omega}\Psi^{HO}d\hat{\Omega}.\end{aligned}$$

Define

$$\hat{D}_g = \frac{\vec{J}_g^{HO} + \frac{1}{3\Sigma_{t,g}} \nabla \phi_g^{HO}}{\phi_g^{HO}}. \tag{3}$$

Note that $\hat{D}$ depends on $\Phi$ through the high order flux and current. The low-order eigenvalue problem is

$$\begin{aligned} \nabla \cdot \quad & \left[ -\tfrac{1}{3\Sigma_{t,g}} \nabla \phi_g + \hat{D}_g \phi_g \right] + (\Sigma_{t,g} - \Sigma_s^{g \to g}) \phi_g \\ & = \textstyle\sum_{g' \neq g} \Sigma_s^{g' \to g} \phi_{g'} + \frac{\chi_g}{k_{eff}} \sum_{g'=1}^{G} \nu \Sigma_{f,g'} \phi_{g'} \end{aligned} \tag{4}$$

If the function $\Phi$ and scalar $k_{eff}$ we used to solve the high-order problem also solve the low-order problem, then we have solved the $k$-eigenvalue problem.

We write (4) as

$$\mathcal{D}\Phi - \mathcal{S}\Phi - \frac{1}{k_{eff}} \chi \mathcal{F}\Phi = 0, \tag{5}$$

where $\mathcal{D}$ is the differential operator and $\mathcal{S}$ the scattering terms. The method proposed in [1]–[3] formulates the eigen-problem as nonlinear equation for $\Phi$ by using

$$k_{eff} = \int \mathcal{F}\Phi \, dV$$

to obtain the equation

$$F(\Phi) = \mathcal{D}\Phi - \mathcal{S}\Phi - \frac{\chi \mathcal{F}\Phi}{\int \mathcal{F}\Phi \, dV} = 0.$$

### A. *Hybrid NDA*

In the results we report in § III, we use the hybrid approach proposed in [1], where a MC simulation is used to solve the scattering-free fixed source high order problem, and thereby compute $\hat{D}$. We motivate this approach in this section.

Traditional methods for computing the dominant eigenvalue of neutron transport equation are deterministic; we employ discretization in space, angle, and energy and solve the eigenvalue problem in discrete space. The discretization of each of these variables can lead to errors which may result in non-physical solutions. Currently, we only concern ourselves with addressing the spatial and angular discretization errors.

The standard spatial discretizations, the diamond difference method or the step-characteristics method, can both be insufficient at times. The diamond difference method is second-order accurate, however, if the mesh is too coarse, this differencing technique can lead to negative fluxes. The step-characteristics method guarantees positive solutions everywhere in the domain, however is only first order accurate [18] The $S_n$ angular discretization can yield "ray effects" or biasing along the discrete angles in our quadrature set [18], [19]. These ray effects can only be remedied by increasing the number of angles in the quadrature set, however this is limited as beyond a certain point the $S_n$ quadrature contains negative weights, leading to instability.

Each of these issues can be avoided entirely by opting to use the MC method. The MC method allows for a continuous treatment of both the spatial and angular variables (and energy, too). While MC simulations have stochastic noise, they have the potential to provide more physically accurate solutions than deterministic methods. Furthermore, these methods are highly parallelizable and their implementation lends itself to emerging computing architectures.

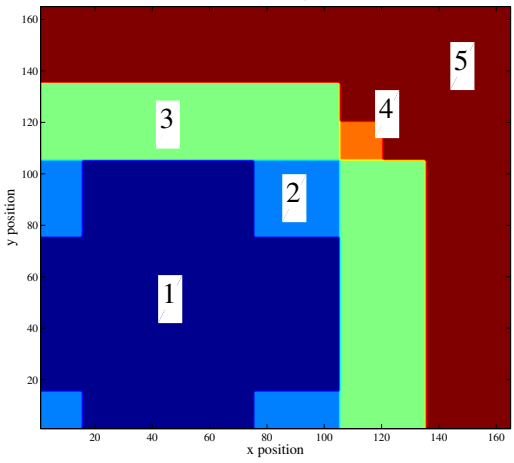
In a pure MC $k$-eigenvalue calculation, one realizes the power method by simulating a sequences of "batches" of particles. The computation begins with an approximation to the fission source, $\mathcal{F}\phi$. Each batch takes as an input a fission source distribution and outputs a new fission source distribution. Once the eigenvector has begun to converge, we begin to average the fission source distributions from each iteration to damp MC noise. The eigenvalue is the ratio of the number of particles born out of fission events from one neutron generation to the next.

In the hybrid method, in which the MC simulation only takes place in order to approximate the inversion of $\mathcal{L}$, we only need to simulate the streaming of particles. All absorption, scattering and fission events are controlled through the low-order system. This allows for a highly simplified implementation of the MC algorithm. The logic is removed almost entirely and particle histories are significantly shorter than traditional MC particle histories.

## III. Results

We report results on the LRA-BWR test problem from [3], [20], [21]. This is a two group, six region problem with five different materials. The system is a 165cm square. We use 1cm square cells in both directions. Figure 1 illustrates the grid and the material distribution.

Figure 1.
Material Layout




The lower-left corner of the domain has a reflective boundary, whereas the remaining boundaries are all vacuum.

Our MC implementation uses Continuous Energy Deposition (CED) tallies [22], which we found to be very efficient in our previous studies [1], [14]. We solve the low-order equation with at Newton iteration. This approach was refered to NDA-NCA in [1], [3], [14].

The code has Matlab and C++ components. The Matlab driver takes the material and domain data and creates the NDA-NCA-MC initial iteration with enough power method iterations to drive the eigen-residual for the lower-order problem to $10^{-3}$ (no more than five). At each NDA-NCA-MC iteration, the driver calls the C++ parallel MC code to simulate particle histories. The C++ code tallies and averages the scalar flux and current which are used to provide a closure for the LO problem. The Matlab driver then reads the scalar flux and current from text files, computes the boundary conditions and builds the discrete low-order problem. At this point, the driver executes a single Newton iteration to update the scalar flux for the next iteration.

The communication between the Matlab driver and the C++ MC code is via file I/O. The driver builds the source term for the MC code from its computed scalar flux and writes it and the domain parameters to a file. The C++ code reads the domain parameters and distributes these to each node. On each node, the source term is read in from the text file and the source, domain parameters and number of histories per thread are distributed to each core via OpenMP. Each core stores an entire copy of the domain configuration and simulates its share of the neutron histories. Each core tallies a copy of the scalar flux and current before collapsing this data to a total, on-node scalar flux and current. We then use a call to MPI_Reduce to compute an average scalar flux and current across cores. Finally, the C++ code writes these data to a file for the driver.

The computations were done on an HP DL585G7 Server running CentOS 6.3 and gcc 4.7.2. Each node has four 1.9 GHZ AMD 6168 twelve-core processors per node with a 512KB cache and 64GB of memory.

In Table I we tabulate weak scaling results of a single transport sweep. This is an accurate surrogate for the full eigensolve, for which the results with fewer nodes require an excessive amount of time.

Table I
WEAK SCALAING OF GROUP 1 TRANSPORT SWEEP

| nodes | time (secs) | speedup |
|---|---|---|
| 1 | 85.1665 | 100.0000 |
| 2 | 85.2150 | 99.9431 |
| 4 | 85.4985 | 99.6117 |
| 8 | 85.6725 | 99.4094 |
| 12 | 85.7175 | 99.3572 |
| 20 | 86.0830 | 98.9353 |

In Figure 2 we plot the results of a strong scaling study for the entire eigensolve, using 10 nodes as the base case. The plot clearly shows that the strong scaling is excellent.

Finally, we plot the results of the solve in Figure 3.

Figure 2. Strong Scaling for Eigensolve

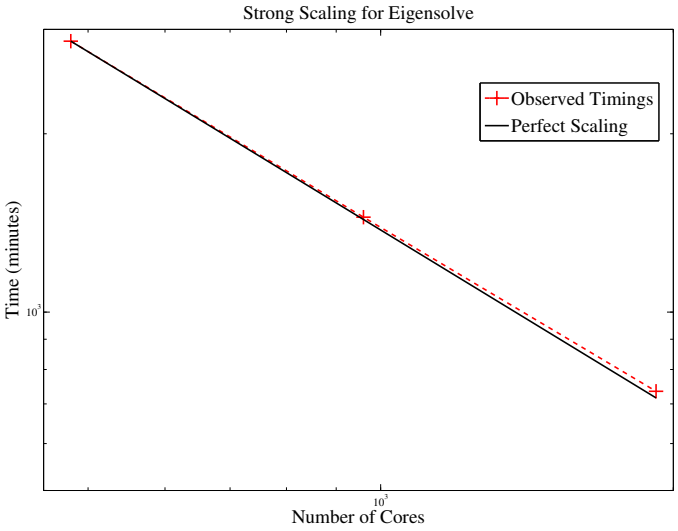
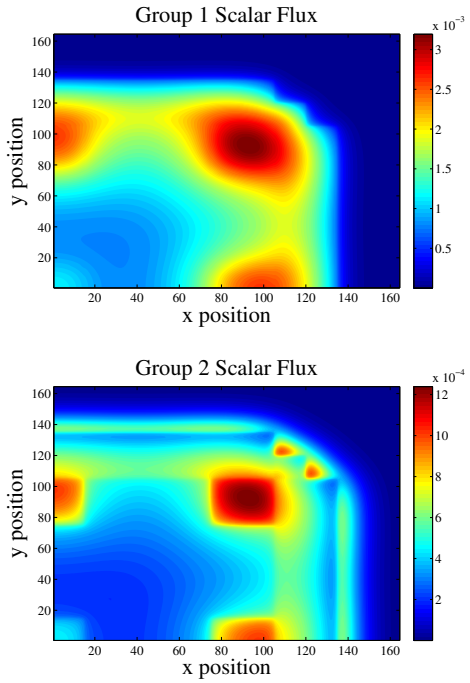



Figure 3. Group Fluxes




## IV. CONCLUSION

In this paper we describe a parallel nonlinear solver for the NDA formulation of the $k$-eigenvalue problem in neutron transport. The solver is a hybrid deterministic/MC method. We demonstrate the method's good scalability properties for a two-dimensional benchmark problem.

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